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On the Interpretation of the level structure of the Ground 3d 5 Manifold of Mn III, Fe IV, Co v and Ni VI

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Abstract

The level structure of the ground 3d 5 configuration of Mn 2+, Fe 3+, Co 4+ and Ni 5+ ions was theoretically interpreted by means of a least-squares fit of the energy parameters to the observed values within the framework of the single-configuration approximation. In the Hamiltonian in addition to real electrostatic, spin-orbit, and spin-spin interactions, electrostatic and spin-orbit interactions correlated by configuration mixing were included. It was shown that the correct positions of almost all the energy levels are determined when the Hamiltonian includes the terms of the lineal (two-body operators) and nonlinear (three-body operators) theory of the configuration interaction. The most correct theoretical description of the experimental spectra was obtained by taking into account relativistic interactions and correlation effects of spin-orbit interactions. Adjustable parameters of the interactions included into the Hamiltonian were found.

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